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Nomenclature Report
Indexes
and
Title-pages

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EDITORIAL REPORT ON NOMENCLATURE, 1955.*

PHYSICAL

Unit of Wave Number.—The use of the symbol κ (Kayser) for cm.$^{-1}$ is optional (cf. Lecomte, *J. Opt. Soc. Amer.*, **1953**, **43**, 410), though rare in Chemical Society publications (cf. *J.*, 1955, 3163; *Ann. Reports*, **1954**, **51**, 12).

Phase Diagrams.—Space can sometimes be saved by abbreviating phase diagrams, as in Figs. *A* and *B* (*J.*, **1955**, **363**, **3056**: cf. also *J.*, 1954, 30).

FIG. *A*.

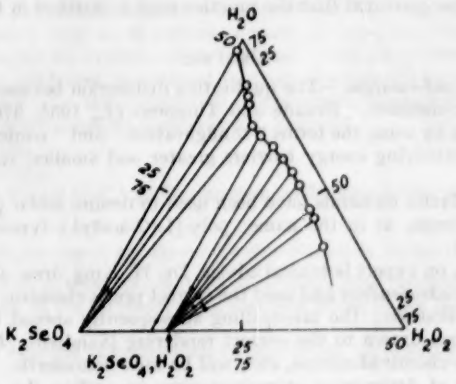
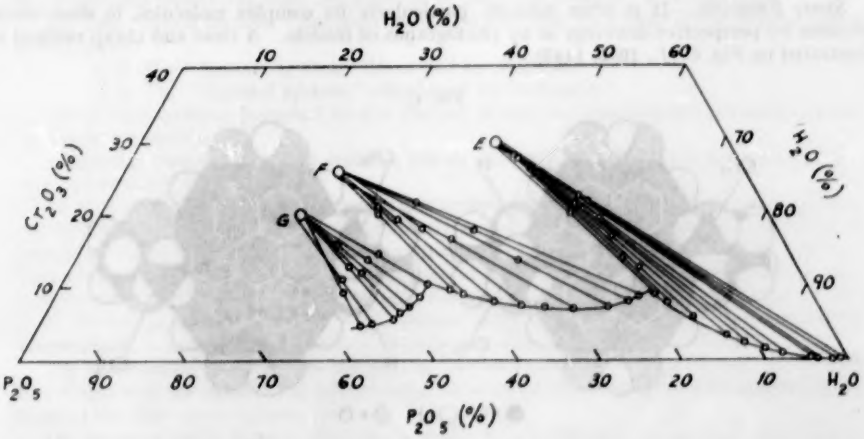


FIG. *B*.



Clarity in Figures.—Detail concerning curves is best printed in the legends and not on the Figures themselves, since too much lettering reduces clarity and spoils the appearance of the curves. An example of the labelling and recording of maxima in infrared spectra is given in *J.*, 1955, 4178.

* Reprints of this Report, and of those for each of the years 1950—54, may be obtained from the General Secretary, The Chemical Society, price 1*s.* each (post free).

Symbol for Molality.—Some confusion has arisen from certain of the Royal Society's recommendations (see *J.*, **1951**, **1677**). The following modifications will be adopted in the Chemical Society's publications:

Units:	molal	m *or* g./kg. of solvent
	molar	M *or* g./l. of solution
Symbols:	concentration (any units)	c or C
	concentration (any units) of a substance X	c_X or C_X
	concentration (molar only) of a substance X	[X]

The only changes involved are: (i) the symbol *m* for molality is abandoned; (ii) c and C may refer to molar, molal, or other units instead of only to the first.

Whenever c, C, c_X, or C_X is used, it must be made clear in the text what units are involved. If several units are involved in one paper, c and C may be used for, *e.g.*, molal and molar units respectively, or *vice versa*, provided that the practice used is clarified in the text.

Organic

Configuration and Conformation.—The qualitative distinction between these two concepts is well known to organic chemists. Braude and Timmons (*J.*, **1955**, **3766**) have given a semi-quantitative distinction by using the terms "configuration" and "conformation" in connexion with stereoisomerism involving energy barriers greater and smaller, respectively, than *ca.* 20 kcal./mole.

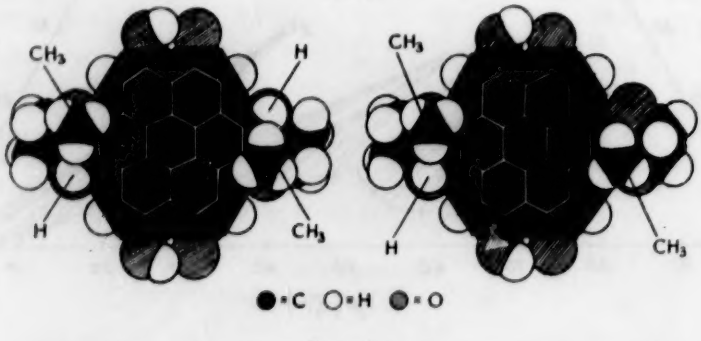
Mixed Polymers.—Prefix numerals have been used to denote molar proportions of the components in mixed polymers, as in the name, poly-[**1**-(*O*-acetyl-L-tyrosine) : **3**-(γ-benzyl-L-glutamate)] (*J.*, **1955**, **232**).

Chondro-.—In **1935**, on expert botanical advice, Dr. H. King drew attention to mis-spelling of the generic name *Chondrodendron* and used the correct prefix chondro- in the names of several derivatives of curare alkaloids; the mis-spelling subsequently spread to the chemical names. Attention has again been drawn to the correct rendering (Sandwith, *Kew Bull.*, **1955**, No. **1**, **58**), and names such as chondrodendrine, etc., will be used henceforth.

Tropane.—Methods of designating stereoisomerism on carbon (by α, β) and on nitrogen (by *a*, *b*) in the tropane series have been devised which may have more general use (for details see *J.*, **1953**, **721**; **1955**, **3504**).

Steric Formulae.—It is often difficult, particularly for complex molecules, to show steric relations by perspective drawings or by photographs of models. A clear and cheap method is illustrated by Fig. *C* (*J.*, **1955**, **1145**).

Fig. *C*.



General

I.U.P.A.C.—The (tentative) rules for nomenclature of inorganic compounds published in *Comptes rendus* of the **17th** (Stockholm) Congress of the International Union of Pure and Applied Chemistry, **1953**, pp. **98**—**119**, were discussed by the Commission of Nomenclature of Inorganic Chemistry at Zürich in **1955**. Comments received on these proposals made further consideration desirable, and the **1953** rules were *not* made definitive at the **1955** meeting.

Extensive revision of older rules for organic nomenclature is in progress, and 100 new rules are due for publication, in tentative form, in the *Comptes rendus* of the Zürich meeting.

I.U.P.A.C. have made available to the organisations adherent to the Union certain proposals, known as the Dyson–Taylor–Patterson system, for the nomenclature of polycyclic compounds. These were unfortunately received too late for inclusion here, but copies may be obtained on application to the Editor, The Chemical Society. Meanwhile we give below the covering letter from the Organic Commission and the Introduction to the system supplied by the Commission :

October 25, 1955.

To Organizations Adherent to the International Union of Pure and Applied Chemistry.

Gentlemen :

You will find enclosed proposals for a new system for naming condensed ring compounds and an introduction to this system. This is known as the Dyson–Taylor–Patterson System and is now being made available, on an experimental basis, to the organizations adherent to the Union. The I.U.P.A.C. Commission on Nomenclature of Organic Chemistry is of the opinion that this system may be of particular value in naming complex structures which cannot be named readily by systems already in use. The proposals in question and the introduction may be published in national journals if so desired by the national organizations. It is requested that any suggestions or comments be sent to Dr. G. M. Dyson, 1 Burton Walks, Loughborough (Leicestershire), England.

Yours very truly,

H. S. Nutting,

Secretary, I.U.P.A.C. Commission on Nomenclature of Organic Chemistry.

Introduction to the Dyson–Taylor–Patterson System

The nomenclature of compounds having condensed ring systems poses two distinct problems : the naming of the structures and the numbering of the positions of the various atoms.

There are several systems of nomenclature now in use for naming and numbering such compounds.

(1) Generally accepted trivial names such as " naphthalene," " phenanthrene," " pyrene," etc., are used for more common compounds. In certain cases, such as anthracene, the traditional numbering does not conform to the more generally accepted rules.

(2) The " fusion method " has been developed and used for a large group of compounds in two ways :

(2.1) The " genetic system," developed by Stelzner.[1]

(2.2) The " skeletal system," developed by Patterson.[2]

(3) A third method, proposed by von Baeyer, is used for compounds not readily named by the fusion system.

In naming very complex ring systems, the results often leave much to be desired in the way of simplicity and clarity.

In 1946 Dr. G. M. Dyson [3] proposed a new system for enumerating cyclic ring structures and in 1948 Dr. F. L. Taylor [4] independently suggested another method by which such structures could be both enumerated and named. Dr. A. M. Patterson [5] modified Dr. Taylor's system in certain respects and suggested that some form of alignment of the two systems would be desirable. Accordingly, the system has been further modified by Dr. G. M. Dyson to its present form. This system, with its new vocabulary and method of enumeration, is so distinctive that it is recognisable wherever it may be used.

The Commission believes that the Dyson–Taylor–Patterson System has real merit and that it probably has outstanding advantages in naming systems which are extremely difficult to name by other methods now available.

On the other hand, there is no evidence before the Commission as yet that this system

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[1] R. Stelzner and H. Kuh, *Literatur-Register der Organischen Chemie*, band **3**, p. 48 (Berlin–Leipzig, 1921).

[2] A. M. Patterson, *J. Amer. Chem. Soc.*, **50**, 3080—4 (1928).

[3] G. M. Dyson, Lecture published by the Royal Institute of Chemistry, October 21, 1946.

[4] F. L. Taylor, *Ind. Eng. Chem.*, **40**, 734—8 (1948).

[5] Personal communication.

will prove generally useful to chemists. Until such evidence is forthcoming, the system cannot be officially recommended by I.U.P.A.C.

Accordingly, the Commission has urged Dr. Dyson to publish this system in its present form, with the hope that chemists will use it in naming unusually complex structures and that they will report back to Dr. Dyson their comments or suggestions. These should be sent to the following address: Dr. G. M. Dyson, 1 Burton Walks, Loughborough, Leicestershire, England.

Infrared Spectra.—On the advice of the Infrared Absorption Data Joint Committee and of the Publication Committee, Council has agreed to discontinue the deposition of copies of infrared spectra with the Society (see *Proceedings*, 1952, 164; *J.*, 1952, 5063) The arrangements for deposition and photocopying were initiated as a temporary expedient, until a more permanent scheme should come into operation. The Chemical Society (and certain other scientific societies) have agreed to support the Anglo-German organisation for the issue of spectra and spectral data on punched cards; the British publishers of these cards are Butterworths Scientific Publications Ltd., 88 Kingsway, London, W.C.2. A description of this punched-card scheme follows this Nomenclature Report; further particulars of it may be obtained from the publishers.

The conditions for publication of infrared spectra in papers published in the *Journal* remain as before (for details see *Proceedings*, 1952, 164), except that spectra which would have been deposited with the Chemical Society will in future be forwarded to the publishers for consideration for the punched-card scheme. Spectra for issue on punched cards need *not* be drawn on the forms obtainable from the Chemical Society, but spectra for publication in the *Journal* must still conform to the requirements given in *Proceedings* (*loc. cit.*).

Spectra already deposited with the Society have been made available for the punched-card scheme. The Society's obligations to supply individual photocopies of these spectra have been taken over by Butterworths Scientific Publications Ltd., to whom application should be made (price 5*s.* per photocopy per spectrum). Individual copies of a spectrum will not be obtainable once that spectrum has been issued on a punched card, for the purpose of the obligation was to make the material available to the scientific public.

The Documentation of Molecular Spectra.

By H. W. Thompson.

During the past fifteen years there has been a marked growth of spectroscopic work in relation to chemical problems. This was stimulated, primarily, by a better theoretical interpretation of the spectra of molecules in terms of the molecular geometry or nuclear structure, and of the molecular energy levels. It led naturally to technical advances in methods of quick, direct, and automatic recording of spectra, so that data on a vast number of molecules have accumulated rapidly. This output of spectral knowledge, already large, is still increasing. There is a particular emphasis on infrared absorption and Raman data, which have become indispensable for much research in organic chemistry involving the study of complex natural or synthetic products. Indeed, the vibrational spectrum of a molecule is now generally recognised as a highly characteristic property, more useful for identification, for assessment of purity, and for other purposes than most other physical properties previously employed. In addition, the spectral data are required in connexion with many physical problems concerned with molecular dynamics.

Anyone working in these fields knows that, for most purposes, it is necessary to have at hand, not only the spectrum of some individual compound, but also a collection of such spectra covering many structural types, for comparison and correlation. The task of making such a collection is formidable, and if carried out by every individual laboratory it would involve an undesirable duplication of effort, if indeed the work could be done effectively at all. Another difficulty arises since rising costs are now making it impossible to publish in the scientific periodicals all the spectra of pure compounds and standard technical products, and many results which might normally be available for general use are accumulating in different laboratories where they lie inaccessible and unknown to the wider circle of potential users.

The compilation of spectral data in a form in which they can be used by different workers to the maximum advantage itself involves some problems. For example, the data are not well suited to tabular presentation, and even if set out in this way they would be very cumbersome. Also, in the case of infrared and Raman spectra, quantitative measures of the band intensities which have absolute significance are, as yet, only rarely available. Whatever method of compiling infrared spectra is adopted, it must be designed so that answers can be quickly obtained to a variety of questions of which the following are examples :

(i) What is the spectrum of a particular compound ?
(ii) With what substance is a measured spectrum associated ?
(iii) What substances give rise to a particular absorption band, or what set of spectral characteristics are connected with some particular atomic grouping or structural feature ?
(iv) What impurities are present in a given substance ?
(v) Which recently published papers deal with some special technical problem ?
(vi) What recent theoretical work has dealt with a particular topic ?
(vii) What were the main points made by a particular author in an important recent paper ?

The most promising kind of catalogue and index for these purposes can be devised by using punched cards, which record the relevant spectral and structural data and can be sorted by means of an appropriate code. The means for setting up such a system have therefore been explored by the Infrared Absorption Data Joint Committee, which was set up several years ago by the Chemical Society to advise on the more general problem of the presentation of spectral data. The following were members of this Committee, representing the bodies indicated :

> H. W. Thompson (Chemical Society and Royal Society, chairman), R. S. Cahn (Editor, Chemical Society), E. D. Hughes and A. E. Martin (Chemical Society), A. C. Menzies (Physical Society), N. Sheppard (Faraday Society), H. Powell (Institute of Petroleum), W. C. Price (Photoelectric Spectrometry Group), J. E. Page (Society of Public Analysts), E. F. G. Herington (Department of Scientific and Industrial Research).

The Committee had the benefit of consultations with a number of those who were potential users, or who had already gained experience with indexes of this kind, including Prof. Sir Alexander R. Todd, Prof. E. R. H. Jones, Dr. H. B. Henbest, Mr. R. Wood [1] (Atomic Weapons

[1] R. Wood, United Kingdom Atomic Energy Authority, AWE Report H26/52.

Research Establishment, Aldermaston), Dr. L. J. Bellamy (Explosives Research and Development Establishment, Waltham Abbey), Prof. E. A. Braude, Prof. J. W. Cook, and Dr. F. L. Rose; a census of views on some points was also taken at meetings of the Infrared Discussion Group and of the Hydrocarbon Research Group of the Institute of Petroleum.

Two kinds of punched card have recently been introduced for spectral data. One is an IBM card, on which the positions of the main absorption bands are shown by slots on a rectangular matrix.[2] These cards, which are being issued by the American Society for Testing Materials, Philadelphia, are sorted by electrically operated Hollerith machines. The other type is a keysort card, prepared under the editorship of Dr. C. Creitz for a Committee of the National Research Council, Washington;[3] this has holes around the edges, coded and slotted according to the spectral and structural characteristics of the compound concerned. These cards are sorted by manual mechanical methods. The main advantage of the IBM cards is that a very large number of cards can be sorted rapidly by the machines. On the other hand, they carry only a limited amount of information, and the inclusion of more would require much larger cards and lead to other difficulties. Keysort cards are able to record much more information, and their main disadvantage is the need for sorting by manual methods. The latter may not, in fact, be a serious shortcoming in the present case, for it is probable that workers in special fields will usually retain groups of cards in defined lots, thus simplifying the sorting operations.

After detailed examination the Committee decided that a scheme involving keysort cards would at present best meet British and European requirements, especially if it could provide rather more information than that furnished by the existing schemes. The extent and kind of material which should be included on the cards, together with detailed methods of coding, were next considered. The Committee was then informed by Dr. H. Kaiser of the Institut für Spektrochemie, Dortmund, about a similar project under his direction sponsored by the Gesellschaft für Spektrochemie und angewandte Spektroskopie. This group, working in conjunction with the Chemisches Zentralblatt in Berlin, planned to provide a literature survey of spectral data on keysort cards, with a code which was more extensive than others used previously, and which was designed specifically to deal with the sort of questions listed above. It became clear that a union of the German scheme, with its literature survey, and the British scheme, which had been directed primarily at the spectra of pure compounds from published and unpublished sources, would be mutually beneficial and might have operational and technical advantages leading to a collection of universal value. The joint plan which has now been agreed upon is outlined below.

General Plan and Coding System. Two identical editions of cards will be published, in English and German respectively, the publishers being Butterworths Scientific Publications, London, and Verlag Chemie, Weinheim. For the present, they will deal only with infrared and Raman spectra, with an emphasis on the former, although it is hoped to extend the scheme later to ultraviolet spectra. Two separate cards will be issued in each edition, namely, S (spectral) and L (literature) cards. S cards will be rose-coloured (infrared spectra) and white (Raman spectra), and the L cards will be yellow. In order to advance from the start along a broad front of the widest possible interest, compounds will be chosen from many classes, such as hydrocarbons, general organic chemicals, fluorocarbons, steroids, carcinogens, heterocyclics, organic derivatives of silicon, phosphorus, and sulphur, pyrimidines, carbohydrates, amides and peptides, polymers, etc. Spectral data will also be included on inorganic materials such as salts and minerals, and on a limited number of standard, technologically important substances of indefinite structure.

(a) *Spectral cards.* The two sides of an S card are illustrated in Figs. 1 and 2. On the front (Fig. 1) the name of the compound is printed, together with its main physical properties, the molecular and structural formulæ, the author or source of the spectrum, and the conditions under which the spectrum was measured. On the reverse side of the card (Fig. 2) the spectrum is shown, with a Table of frequencies of the chief bands and their rough apparent intensities. The infrared spectra are drawn on a standard format with abscissa linear in wave numbers, covering the range 200—4000 cm.$^{-1}$. A break of scale is made at 2000 cm.$^{-1}$, and the positive ordinate is percentage transmittance.

Around the edges of the card there are two rows of holes, with 203 holes in all. These can be cut so as to make deep, shallow, or " middle " slots. The upper and right-hand sides (Figs. 1 and 2, 1—31 and a—v) are used for coding the structural features of the compound, and the bottom and left-hand sides (32—61 and A—V) are used for marking the positions of the main

[2] L. E. Kuentzel, *Analyt. Chem.*, 1951, **23**, 1413.
[3] See W. Brugel, " Einführung in die Ultrarotspektroskopie," Steinkopff, Darmstadt, 1954, pp. 224—226.

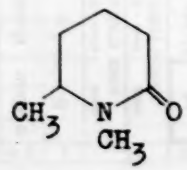
$C_7H_{13}ON$

MOL. WT. 127.2

AUTH.CODE /YEAR EDW-0-SIN/54

LIT. CARD NO.

BEILSTEIN SYSTEM NO. 3179



1:6-Dimethylpiperid-2-one

m.p

b.p. 80-85°

STATE liquid

SPECTRAL RANGE 600-3600cm^{-1}

d

CONC.,PRESS.,TEMP.

PRISM / EXCITING LINE NaCl

n_D^{24} 1.4802

THICKNESS film

APPARATUS P. E. 21

PURITY elem. anal.

DIFFERENTIAL

AUTHOR O. E. Edwards and Tara Singh

JOURNAL Canad. J. Chem. 32. (1954.) 683-91

	DEEP	MIDDLE	SHALLOW
I	HYDRO. CARBON	HETEROCYCLIC NUCLEUS	OVERLAP
-X	-Cl	-I, -IO$_n$	-Br
	-CN	-NCO, -NC, -SCN, -N$_3$	-F
	-NO$_2$	NITRAMINE, NITROSAMINE	-NO
-X-	-O-	ACETAL, OZONIDE ORTHOESTER	-S-
	-(SO$_2$)-	-X<(O, S, Se)	-(SO)-
	-N=N-, -N=(NO)-	=N$_2$	-P<
-X-Z	-N<	-X<(N, P, As)	-(XO)$_n$<(N,P,As)
-Z	-H (c-c)	-OR', -SR'	-H (c=c)
	-R (c-c)	-NR$'_2$, -Hal.	-R (c=c)
II -U [Y]	-V [O]	-V [N-T]	-V [S]
	-R [O]	-R [N-T]	-R [S]
U C Y V -V	-R	T: -R, -H; CYCL. KETONE	-H
	-OH, -OOR', -SH, -OM	T: -OH; CYCL. ANHYDRIDE	-OCOR'
	-OR'	T: -OR'; LACTONE	-SR'
	-NR$'_2$	T: -NR$'_2$; LACTAM	-Hal., -N$_3$

SUBSTITUENT CONJUGATED TO DOUBLE BOND			
	IN RING	AT RING	IN CHAIN
1000 11/55	BETAINE, MESOION COMPD.	ISOTOPE	MOLECULAR COMPOUND
	MINERAL ACID DERIV., ALCOHOLATE	RADICAL COMPLEX	METALLORGANIC COMPOUND

poly I

CODE NO 222 BUTTERWORTHS, LONDON, VERLAG CHEMIE WEINHEIM COPYRIGHT 1956

FIG. 1.

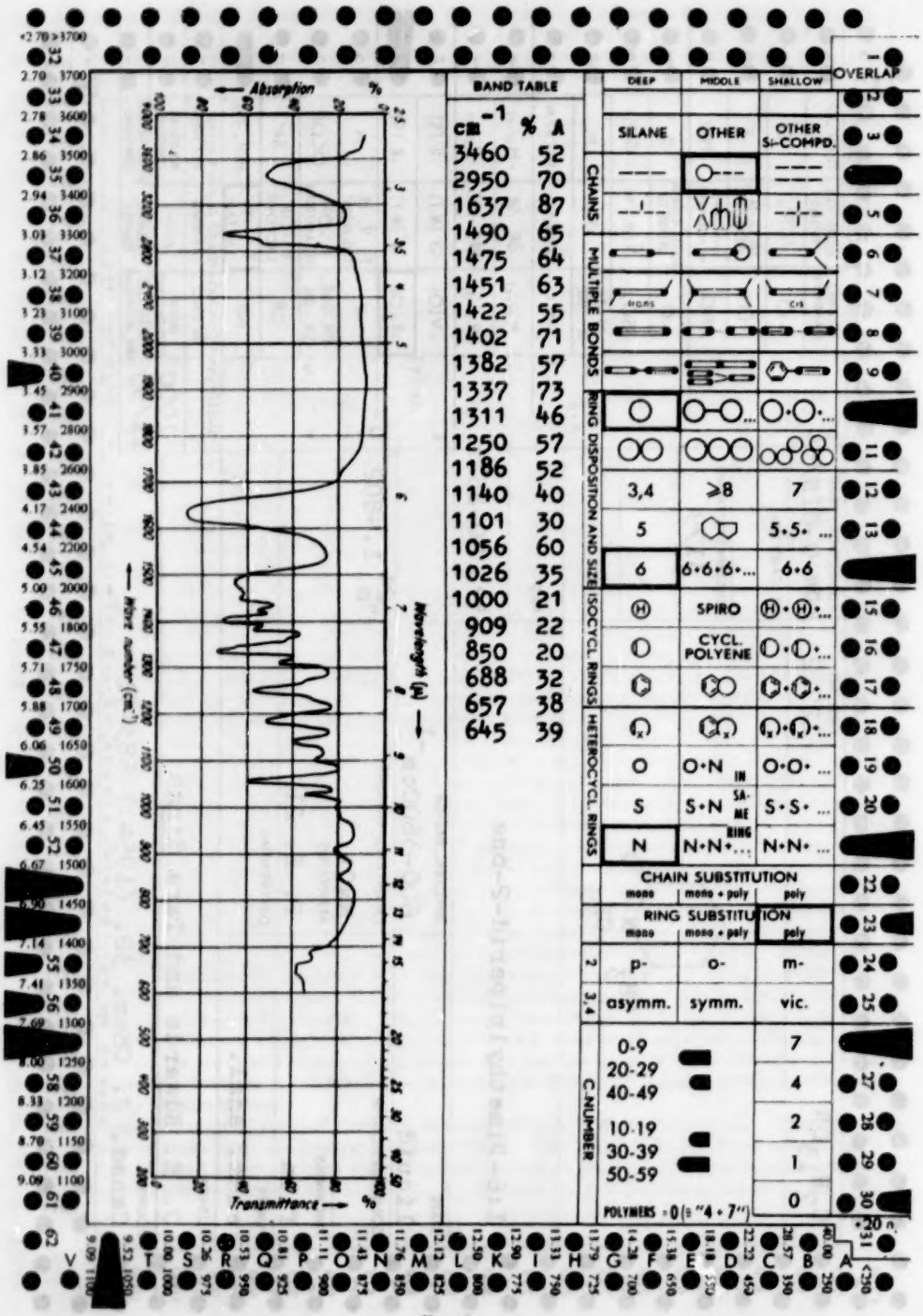

Absorption
Transmittance
Wave number (cm⁻¹)
Wavelength (μ)
BAND TABLE
cm⁻¹ % A
3460 52
2950 70
1637 87
1490 65
1475 64
1451 63
1422 55
1402 71
1382 57
1337 73
1311 46
1250 57
1186 52
1140 40
1101 30
1056 60
1026 35
1000 21
909 22
850 20
688 32
657 38
645 39
DEEP
MIDDLE
SHALLOW
OVERLAP
SILANE
OTHER
OTHER Si-COMPD.
CHAINS
MULTIPLE BONDS
trans
cis
RING DISPOSITION AND SIZE
3,4
≥8
7
5
5·5·...
6
6·6·6·...
6·6
ISOCYCL. RINGS
SPIRO
CYCL. POLYENE
HETEROCYCL. RINGS
O
O·N IN SAME RING
O·O·...
S
S·N IN SAME RING
S·S·...
N
N·N·...
N·N·...
CHAIN SUBSTITUTION
mono
mono + poly
poly
RING SUBSTITUTION
mono
mono + poly
poly
2
p-
o-
m-
3,4
asymm.
symm.
vic.
C-NUMBER
0-9
20-29
40-49
10-19
30-39
50-59
7
4
2
1
0
POLYMERS = 0 (= "4 + 7")

FIG. 2.

bands, up to eight or ten strong bands being marked. The decision as to which bands should be chosen as being the most significant from a spectroscopic standpoint is difficult, since for some purposes the weaker bands may be more informative than the stronger. For this reason, therefore, it is proposed at first to indicate by black markings the holes which should be slotted according to the present system, but not to cut the slots. This will enable any user who prefers to use another system of slotting, which may be more appropriate to his special needs, to do so. The spectral cards are also linked to the literature cards, where relevant, by a defined code.

The code used to record the structural characteristics has been designed to cater for all likely organic compounds, and is therefore necessarily somewhat elaborate. It will be described in detail in a manual supplied to subscribers, and also in a handy abridged form for day-to-day use. It is based upon four structural features of the compound, namely, the number of carbon atoms, the basic skeleton, and the types and positions of substituent groups. The molecule is

Some examples of coding.

d = deep, s = shallow, m = middle slotting.

I, Chloromycetin. II, Strychnine. III, Sulphathiazole.
IV, *isopseudo*Irone. V, *N*-Benzyloxycarbonyl-*O*-D-glycyl-DL-serine hydrochloride.
VI, 3-Cyano-4-ethoxymethyl-2-hydroxy-6-methyl-5-nitropyridine.
VII, Acetic acid. VIII, Tigogenin acetate.

Number of carbon atoms.

Hole no.	26	27	28	29	30	31
I				s	d	
II				d	s	s
III	d		s			
IV		s			d	
V			s	d		
VI	s	d				
VII			d		s	
VIII	d		s			s

Basic skeleton.

Hole no.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
I										d				d			d					s		d	
II	s				m						s	s	s	m	d		d	s	d		s		d		
III									d	s			d	d			d	d		m			m	d	
IV	s				d	s	d	m	d													d			
V										d				d			d					m	d		
VI				m					d	d				d				d			d	d	s		
VII				d																		d			
VIII	s			m	m					m	s		s	m	m				s			d	s		

Substituents.

Hole no.	a	b	c	d	e	f	g	h	i	k	l	m	n	o	p	q	r	s	t	u	v
I	s		d		d	d				d			d				d	d			
II													d				m				
III							d		d	s	m							d			
IV													d	d				s			
V									m	d		d	d		d	d	d				
VI				d	d	d				s	d							d			
VII													d		d						
VIII						m					d		d			d					

regarded as being built up from structural units, which have been selected, as far as possible, to possess chemical and spectroscopic significance. For example, the basic skeleton may be characterised (holes 4—21) by the degree of branching or of unsaturation of a carbon chain, by the number and size of rings—fused or unfused—by the presence of hetero-atoms in a ring, or by the

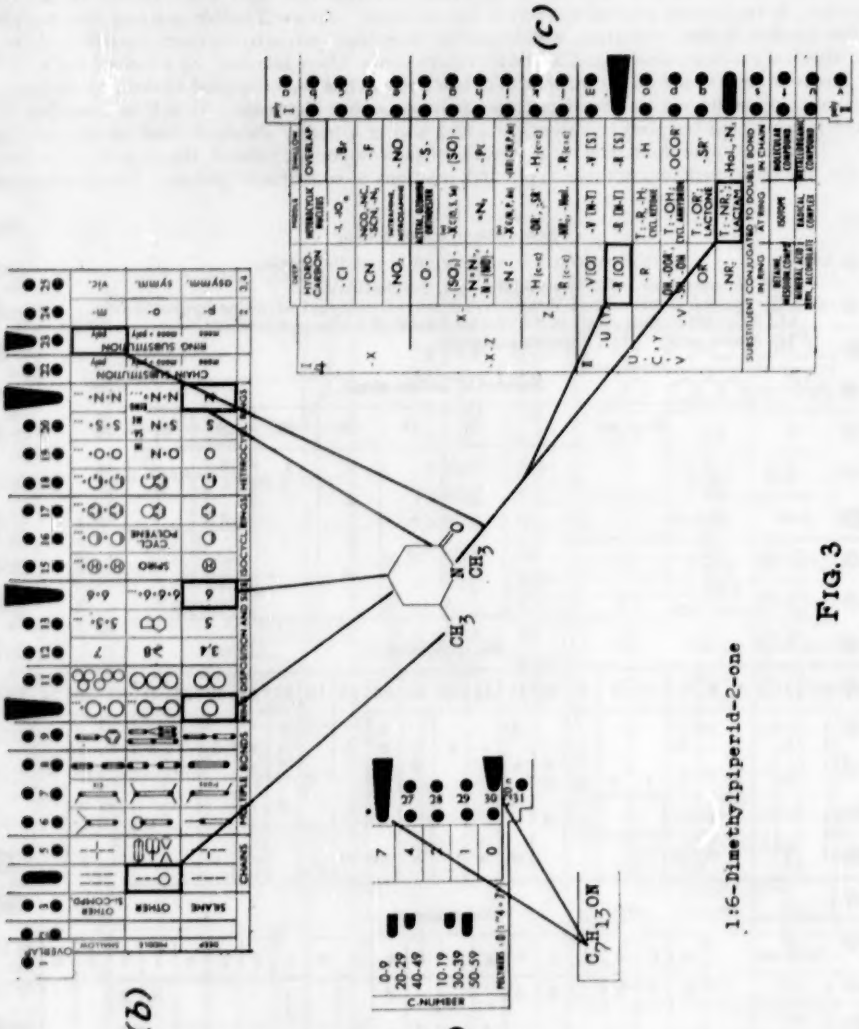
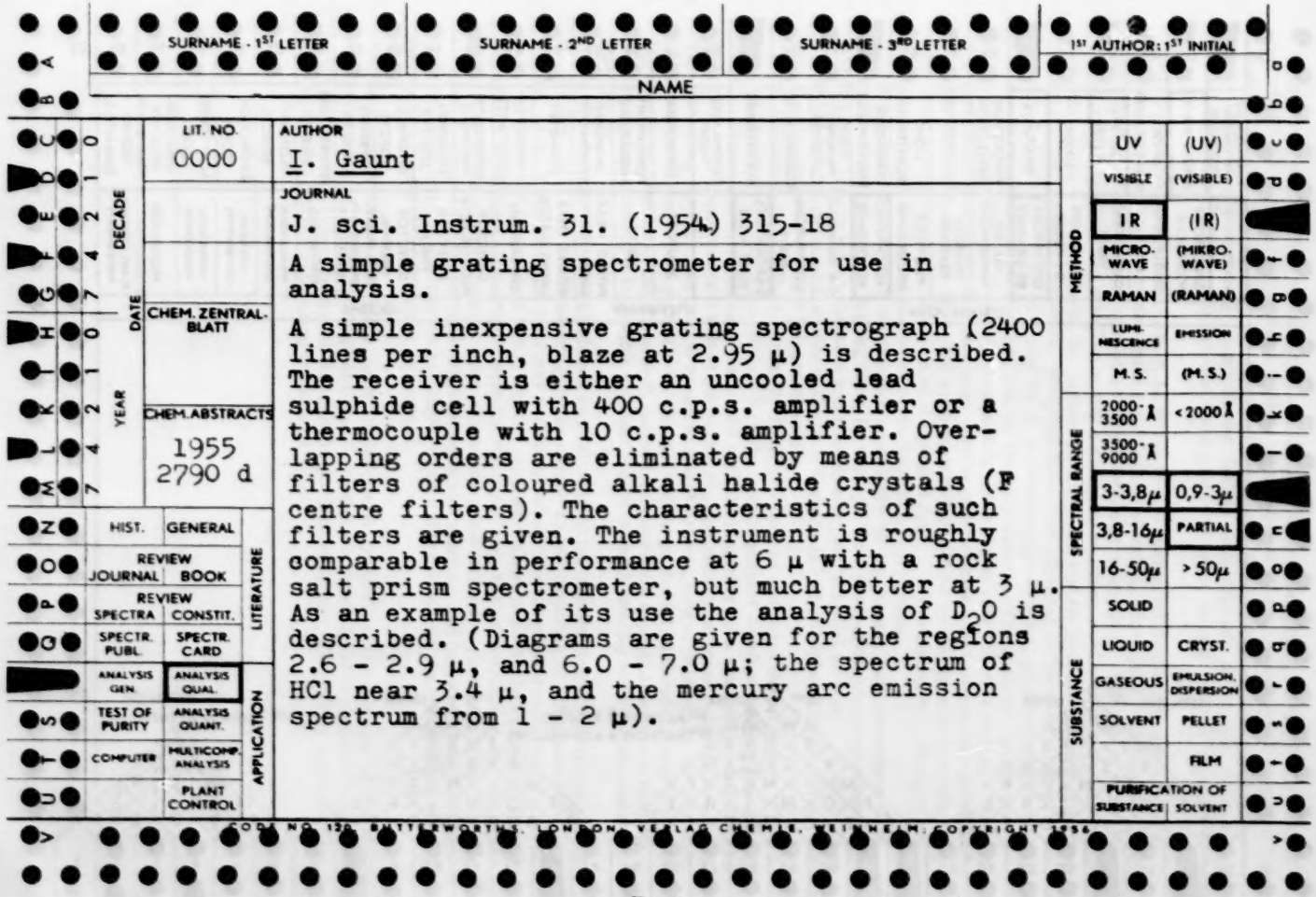


FIG. 3

1:6-Dimethylpiperid-2-one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AUTHOR
I. Gaunt
JOURNAL
J. sci. Instrum. 31. (1954) 315-18
CHEM. ZENTRAL-BLATT
CHEM. ABSTRACTS
1955
2790 d
A simple grating spectrometer for use in analysis.
A simple inexpensive grating spectrograph (2400 lines per inch, blaze at 2.95 μ) is described. The receiver is either an uncooled lead sulphide cell with 400 c.p.s. amplifier or a thermocouple with 10 c.p.s. amplifier. Overlapping orders are eliminated by means of filters of coloured alkali halide crystals (F centre filters). The characteristics of such filters are given. The instrument is roughly comparable in performance at 6 μ with a rock salt prism spectrometer, but much better at 3 μ. As an example of its use the analysis of D_2O is described. (Diagrams are given for the regions 2.6 - 2.9 μ, and 6.0 - 7.0 μ; the spectrum of HCl near 3.4 μ, and the mercury arc emission spectrum from 1 - 2 μ).
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METHOD
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(UV)
VISIBLE
(VISIBLE)
IR
(IR)
MICRO-WAVE
(MIKRO-WAVE)
RAMAN
(RAMAN)
LUMI-NESCENCE
EMISSION
M.S.
(M.S.)
SPECTRAL RANGE
2000-3500 Å
< 2000 Å
3500-9000 Å
3-3,8μ
0,9-3μ
3,8-16μ
PARTIAL
16-50μ
> 50μ
SUBSTANCE
SOLID
LIQUID
CRYST.
GASEOUS
EMULSION, DISPERSION
SOLVENT
PELLET
FILM
PURIFICATION OF SUBSTANCE
SOLVENT
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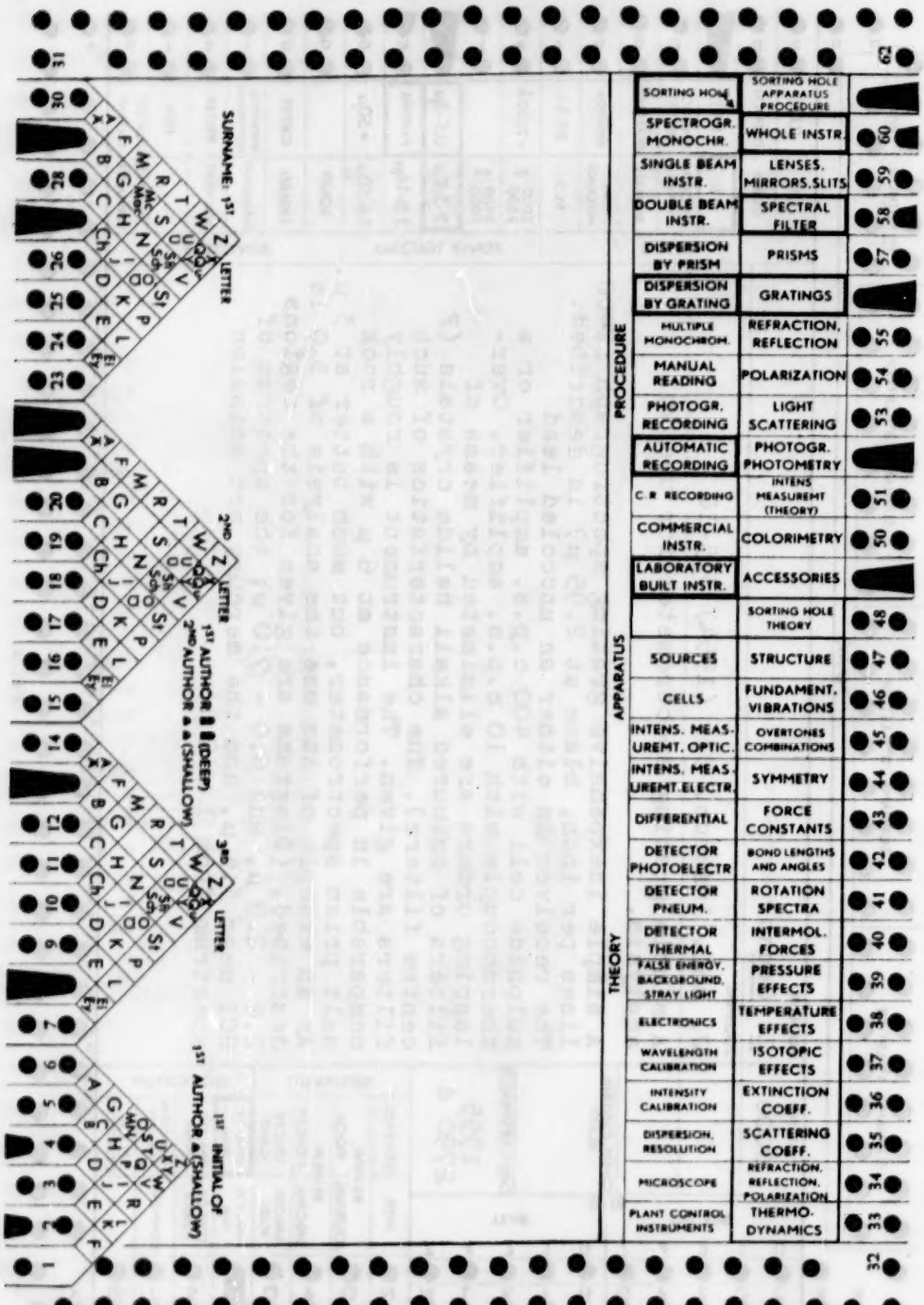
FIG. 4.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PROCEDURE
APPARATUS
THEORY
SORTING HOLE
SORTING HOLE APPARATUS PROCEDURE
SPECTROGR. MONOCHR.
WHOLE INSTR.
SINGLE BEAM INSTR.
LENSES, MIRRORS, SLITS
DOUBLE BEAM INSTR.
SPECTRAL FILTER
DISPERSION BY PRISM
PRISMS
DISPERSION BY GRATING
GRATINGS
MULTIPLE MONOCHROM.
REFRACTION, REFLECTION
MANUAL READING
POLARIZATION
PHOTOGR. RECORDING
LIGHT SCATTERING
AUTOMATIC RECORDING
PHOTOGR. PHOTOMETRY
C.R. RECORDING
INTENS MEASUREMT (THEORY)
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DIFFERENTIAL
FORCE CONSTANTS
DETECTOR PHOTOELECTR
BOND LENGTHS AND ANGLES
DETECTOR PNEUM.
ROTATION SPECTRA
DETECTOR THERMAL
INTERMOL. FORCES
FALSE ENERGY, BACKGROUND, STRAY LIGHT
PRESSURE EFFECTS
ELECTRONICS
TEMPERATURE EFFECTS
WAVELENGTH CALIBRATION
ISOTOPIC EFFECTS
INTENSITY CALIBRATION
EXTINCTION COEFF.
DISPERSION, RESOLUTION
SCATTERING COEFF.
MICROSCOPE
REFRACTION, REFLECTION, POLARIZATION
PLANT CONTROL INSTRUMENTS
THERMO-DYNAMICS

FIG. 5.

presence of exocyclic double bonds. The positions of substituent groups (holes 22—24) are indicated, for example, for the various possible arrangements around a ring system, and for *cis-trans*-isomers. Designation of the nature of substituent groups (holes a—s) requires a rather more intricate coding system, especially for dealing with aliphatic structures. It has been found convenient to distinguish between three structural types, namely $-X$, $-X-Z$, and $U-\underset{\underset{Y}{|}}{C}-V$ and by specifying the groups X, Y, Z, U, and V to characterise all classes of compound, or parts of a compound. The cards also make provision for recording other classes such as molecular compounds, radicals, isotopic species, and organometallic compounds. The use of three kinds of slot—deep, shallow, and middle—makes it necessary to follow certain rules and priorities in sorting. Thus, deep slots have the highest priority, and middle slots the lowest. The most important and commonly occurring groupings have been allocated to the deep slots.

Fig. 3 shows the coding of a card for 1 : 6-dimethylpiperid-2-one, (*a*) shows the number of carbon atoms, (*b*) the basic skeleton, and (*c*) the substituents. The annexed Table shows how the coding is applied to a number of compounds belonging to very different classes. The code has been tested as a whole on a very large number of substances, and will certainly prove satisfactory. However, it is possible that some users will prefer for special reasons to employ their own code, or make some modification of the present one. For this reason too, the holes which should be slotted will be marked on all cards, but not cut at present.

Certain substances cannot be classified completely by the present code, sometimes because their structure is indefinite. Among these, for example, are a number of natural substances with trivial names, certain mixed polymers and condensates, and technical solvents. In such cases a card will be used on which the code to the basic skeleton (1—25) is replaced by an alphabetical key, the remainder of the card being unaltered.

(b) *Literature cards.* The L cards, the front and back of which are shown in Figs. 4 and 5, may relate either to spectra recorded on S cards, or to important developments of technique or theory. Where relevant, the S and the L card are linked together by a cross-reference. On the front face of the L cards there is a short abstract of the publication concerned, with full references. The holes along the edges are used to record names of authors, year of publication, an indication of the nature of the work (*e.g.*, analysis), the spectral range studied, the state of aggregation of the sample, and details of the equipment, method, or theoretical aspects discussed in the paper. By appropriate slotting, it is possible to select a card or cards dealing with specific matters of these kinds.

(c) *Blank cards.* The above code is of general value for the classification of organic compounds on punched cards and would naturally be applicable to the recording of other molecular properties. Also, some spectroscopists may wish to introduce into the present collection of spectral cards certain other data of their own. For this purpose, arrangements are being made to furnish subscribers with blank cards printed with the structural code but otherwise carrying no specific data. For instance, there may be cases where very small shifts of a particular band, say of a carbonyl group in a series of compounds, are highly characteristic and important in some laboratory, and such small shifts may be too slight to be differentiated on the standard cards. In such cases a refined set could easily be prepared.

The Infrared Absorption Data Joint Committee is grateful to the German group, and especially to Drs. H. Kaiser, G. Bergmann, and G. Kresze, for their helpful co-operation, and also to the publishers. It is to be hoped that this Anglo-German scheme will provide a satisfactory basis for a wider international usage in the near future.

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ERRATA

1951, page 1384, line 30. *For* King, *J.*, 1948, 1820 *read* King, *J.*, 1949, 1817.

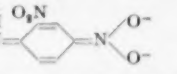
1951, page 2966, line 25*. *For* m. p. 129° *read* m. p. 189°.

1951, page 3296, line 18. *For* 3 g. *read* 10 g.

1953, page 1080, Table. For (14)2″-*Methoxy-5-2-pyridyl* read (14)2″-*Methoxy-5-3′-pyridyl*.

1953, page 2219. In the second set of three formula all the groups -CH- *should read* =CH—.

Formula (II) *should read*



1954, page 383. The arrows between formulae (X) and (XII) should be reversed.

1954, page 1572, line 7*.
1954, page 1573, line 10*, 4*.
1954, page 1574, line 3, 5*.
1954, page 1575, line 11*.
1954, page 1576, line 22, 25, 29, 13*, 6*.
1954, page 1577, line 3.

} Compounds should be named as substituted propyloxybenzenes and not as substituted propylbenzenes.

1954, page 1700, line 17*. *For* 2·16 *read* 1·83.

1954, page 1700, line 17*. *For* 1·98 *read* 1·30.

1954, page 2117, Table 3, line 1. *For* 114 *read* 144.

1954, page 3129, line 9*. *For* latter *read* former.

1954, page 3808, line 14. *For* 3024—3058 *read* 3042—3058.

1954, page 4476, line 2*. *For* Miller *read* Millar.

1954, page 4587, Summary, line 3. *For* 5 : 3′ : 5′-trihydroxy- *read* 5 : 2′ : 5′-trihydroxy-.

1955, page 189, line 18*. *For* Hott-Jorgensen *read* Hoff-Jorgensen.

1955, page 317, line 6*. *For* final *read* thermal.

1955, page 516, line 20. *For* 210° *read* 120°.

1955, page 583, lines 13, 14. *For* Found : C, 19·9; H, 3·2. Calc. for $(C_6H_{14}O_6P)_2Ba$: C, 20·2; H, 3·4% *read* Found : P, 8·4. Calc. for $C_6H_{14}O_6PBa$: P, 8·5%.

1955, page 628, line 13*. For *J.*, 1936, 51 read *J.*, 1936, 231.

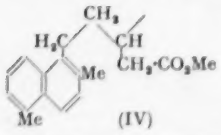
1955, page 628. Equation at bottom of page *should read* $x = (h_1/h_2) \ln \{[(h_1/h_2) + b]/[(h_1/h_2) + b - x]\}$.

1955, page 630. Table in centre of page. *For* $[HO_3^+]$ *read* $[H_3O^+]$.

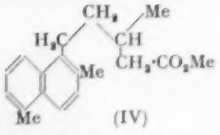
* From bottom of main text.

Errata.

1955, page 659. *For*



(IV) *read*

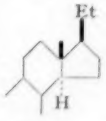


(IV)

1955, page 691, line 2*. *For* 3β-aminocholest-5-ene *read* 3β-methylaminocholest-5-ene.

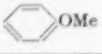
1955, page 699, formula (XXXVI). *For* Me_2N *read* Me_3N.

1955, page 699, formulae (XLIX) and (L). Rings C and D *should read*

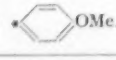


1955, page 804, line 23. *For* diazo*cyclo*butane *read* diaza*cyclo*butane.

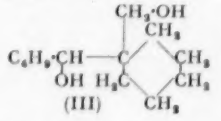
1955, page 1404, Equation (I), right-hand side. *For*



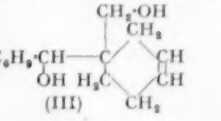
read



1955, page 1463. *For*



read



1955, page 1749, Summary, lines 2 and 3. *Delete* and decafluoro*cyclo*hexane.

1955, page 1854, formula (VIII). A positive charge should be attached to the quaternary nitrogen atom.

1955, page 2535, line 33. *For* 0·01N- *read* N- or 0·1N-.

1955, page 2535, line 34. *For* 260 mμ *read* 246 mμ.

1955, page 2573. The left-hand Figure should be numbered 4, the right-hand Figure 5. The captions remain as printed.

1955, page 2689, line 34. *For* m. p. 167·5° *read* m. p. 267·5°.

1955, page 2691, line 20*. *For* the other monohydroxylated dihydropteridine *read* any other monohydroxylated pteridine.

1955, page 2729, Fig. 4. Legend should read : *A*, P_{O_2}; *B*, P_{CO}; *C*, P_T.

1955, page 2737, line 9*. *For* The *read* An.

1955, page 2737, line 8*. *For* shows *read* showed.

1955, page 2740, line 13*. *For* consistent *read* constant.

1955, page 2938, Table 1, Col. 7, 2nd entry. *For* -3×10^7 *read* $\sim 3 \times 10^7$.

1955, page 2949, formula (IX). *The two groups marked* CH *should read* CH_2.

1955, page 2989, line 14. *For* Groves *read* Gardner, Grove, and Ismay.

1955, page 3010, lines 5—6. *For* L-cystine-3-phenylhydantoin (I) *read* L-cystinebis-3-phenylhydantoin (II).

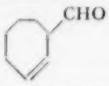
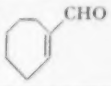
* From bottom of main text.

Errata.

1955, page 3070, Table 2. Column headed X (Å) *should read*

0·722
1·858
0·281
0·631
−0·184
0·178
3·233
−0·084

1955, page 3320, line 16. *For* a decrease in the dielectric *read* an increase in the dielectric.

1955, page 3335, Table. *For*  *read* 

1955, page 3411, line 7. Equation (ii) should read $I/t = k_1^\circ - a^\circ(J/t)$.

1955, 3501, line 20. *For* water *read* 2N-hydrochloric acid.

1955, page 3700, line 3. *For* mole^{-1} kfl. *read* mole^{-1} kg.

1955, page 3715, line 23. *For* $\mathrm{d}V/\mathrm{d}t$ *read* $\mathrm{d}v/\mathrm{d}t$.

1955, page 3716, footnote, line 1. *For* Discussion section *read* Faraday Society Discussion.

1955, page 3717, line 2*. *Before* turns of the spiral *add* distance between the.

1955, page 3720, line 17. *For* $2{\cdot}5/x_1 \times 10^{-1}$ *read* $2{\cdot}5x_1 \times 10^{-4}$.

1955, Plate facing page 3764, Figs. 2 and 3. The captions should be interchanged.

1955, page 3781, line 18*. *For* (as I, Y = $CH_2{\cdot}\overset{+}{N}HPh{\cdot}CH_2$) *read* (as I, Y = $CH_2{\cdot}\overset{+}{N} < C_5H_{10}{\cdot}CH_2$).

1955, page 3781, line 9*. *For* (as I, Y = $CH_2{\cdot}\overset{+}{As}HPh{\cdot}CH_2$) *read* (as I, Y = $CH_2{\cdot}\overset{+}{As}MePh{\cdot}CH_2$).

1955, page 3781, line 4*. *For* (as I, Y = $\overset{+}{As}HPh$ and $\overset{+}{Sb}HPh$) *read* (as I, Y = $As{\cdot}C_6H_4Me$ and $Sb{\cdot}C_6H_4Me$).

1955, page 3887, lines 2, 12, 17. *For* $C_4Cl_4F_6$ *read* $C_4Cl_4F_4$.

1955, page 3887, line 27. *For* Found : C, 20·6; Cl, 30·7%; *M*, 233. Calc. for $C_4Cl_2F_6$: C, 20·6; Cl, 30·5%; *M*, 233 *read* Found : C, 24·8; Cl, 36·2%; *M*, 195. Calc. for $C_4Cl_2F_4$: C, 24·6; Cl, 36·4%; *M*, 195.

1955, page 3888, line 2. *For* Found : C, 20·4; Cl, 30·0%; *M*, 233. $C_4Cl_2F_4$ requires C, 20·6; Cl, 30·5%; *M*, 233 *read* Found : C, 24·6; Cl, 36·0%; *M*, 195. $C_4Cl_2F_4$ requires C, 24·6; Cl, 36·4%; *M*, 195.

1955, page 4154, formula (III). In the right-hand benzene ring, R″ *should read R′*.

1955, page 4169, introduction, line 8. *For* bis-2 : 2 : 2-trifluoromethylamine *read* bis-2 : 2 : 2-trifluoroethylamine.

1955, page 4180, line 5. *For* Fig. 2*g read* Fig. 2, VII.

1955, pages 4435—4439. *For* diphenylbenzoquinone *read* diphenoquinone *throughout*.

1955, page 4473, formula (XIII). *For* *read*

1955, page 4473. *For* phoshine *read* phosphine.

* From bottom of main text.

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